

CLAIMS:

1. A compound having the structural formula  $L^1[MQ^1Q^2]L^2$  in which M is a mid-transition metal selected from the group consisting of Nb, Ta, Mo, W, Mn and Re,  $Q^1$  and  $Q^2$  are each a univalent radical, and  $L^1$  and  $L^2$  are ligands coordinated to M, wherein each of  $L^1$  and  $L^2$  contains a first coordinating atom that is a nitrogen atom contained within a C=N group, and a second coordinating atom that is either a second nitrogen atom, optionally present in a second C=N group, or an oxygen, sulfur or phosphorus atom.

2. The compound of claim 1, wherein, in each of  $L^1$  and  $L^2$ , the second coordinating atom is a second nitrogen atom.

3. The compound of claim 2, wherein, in each of  $L^1$  and  $L^2$ , the second nitrogen atom is present in a second C=N group.

4. The compound of claim 3, wherein  $L^1$  and  $L^2$  are identical.

5. The compound of claim 4, wherein the first nitrogen atom in each of  $L^1$  and  $L^2$  is bound to a first substituent  $R_S$ , and the second nitrogen atom in each of  $L^1$  and  $L^2$  is bound to a second substituent  $R_L$ , wherein the difference in steric bulk between  $R_S$  and  $R_L$  is sufficient to result in isospecificity when the compound is used as a polymerization catalyst.

6. The compound of claim 3, wherein  $L^1$  and  $L^2$  are different.

7. The compound of claim 6, wherein the first and second nitrogen atoms in the ligand  $L^1$  are bound to a first substituent  $R_S$ , and the first and second nitrogen atoms in the ligand  $L^2$  are bound to a second substituent  $R_L$ , wherein the difference in steric bulk between  $R_S$

and  $R_L$  is sufficient to result in syndiospecificity when the compound is used as a polymerization catalyst.

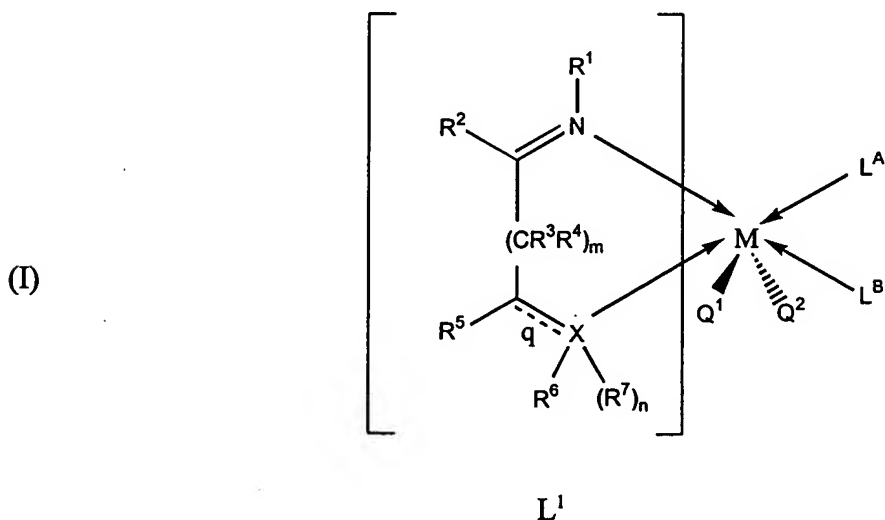
8. The compound of claim 1, wherein the compound has a positive charge  $+y$  and is associated with  $y/z$  anions each bearing a negative charge  $-z$ .

9. The compound of claim 8, wherein  $y$  and  $z$  are independently integers in the range of 1 to 4 inclusive.

10. The compound of claim 9, wherein  $y$  and  $z$  are independently 1 or 2.

11. The compound of claim 8, wherein the anions are selected from the group consisting of halide and pseudohalide.

12. A compound having the structure of formula (I)



wherein:

$M$  is a mid-transition metal;

Q<sup>1</sup> and Q<sup>2</sup> are independently selected from the group consisting of hydrido, halide, alkoxy, amido, unsubstituted C<sub>1</sub>-C<sub>30</sub> hydrocarbyl, C<sub>1</sub>-C<sub>30</sub> hydrocarbyl substituted with one or more substituents such as electron-withdrawing groups, and C<sub>1</sub>-C<sub>30</sub> hydrocarbyl-substituted Group IVB elements, or Q<sup>1</sup> and Q<sup>2</sup> may together form an alkylidene olefin, acetylene, or a five-  
5 or six-membered cyclic hydrocarbyl group;

m and n are independently zero or 1;

q is an optional double bond;

X is N, O, S or P, with the provisos that (a) when X is N or P, then either n is 1 or q is present as a double bond, but not both, and (b) when X is O or S, then n is zero and q is absent;

10 R<sup>1</sup>, R<sup>6</sup>, and R<sup>7</sup> are independently hydrido, hydrocarbyl or substituted hydrocarbyl, and R<sup>2</sup> and R<sup>5</sup> are independently hydrido, halo, hydrocarbyl or substituted hydrocarbyl, or R<sup>1</sup> and R<sup>2</sup> and/or R<sup>5</sup> and R<sup>6</sup> may be taken together to form a linkage -Q-, resulting in a five- or six-membered ring, wherein Q is -[(CR)<sub>a</sub>(Z)<sub>b</sub>]- in which a is 2, 3 or 4, Z is N, O or S, b is zero or 1, the sum of a and b is 3 or 4, and R is selected from the group consisting of hydrido, halo,  
15 hydrocarbyl, hydrocarbyloxy, trialkylsilyl, NR<sup>8</sup><sub>2</sub>, OR<sup>9</sup>, and NO<sub>2</sub>, wherein R<sup>8</sup> and R<sup>9</sup> are each independently hydrocarbyl, or wherein R moieties on adjacent carbon atoms may be linked to form an additional five- or six-membered ring, or R<sup>2</sup> and R<sup>5</sup> may together form a linkage -Q- as just defined;

20 R<sup>3</sup> and R<sup>4</sup> are independently selected from the group consisting of hydrido and hydrocarbyl, or at least one of R<sup>3</sup> and R<sup>4</sup> may be bound through a lower alkylene linkage to an atom contained within L<sup>A</sup> or L<sup>B</sup>;

L<sup>A</sup> and L<sup>B</sup> are ligands which may be the same or different and are independently selected from the group consisting of nitrogen-containing, sulfur-containing and oxygen-containing heterocycles, tertiary amines and phosphines, or L<sup>A</sup> and L<sup>B</sup> may together form a  
25 single bidentate ligand that may or may not be the same as L<sup>1</sup>,

with the proviso that when (a) L<sup>A</sup> and L<sup>B</sup> form a single bidentate ligand that is identical to L<sup>1</sup> and M is V or Cr, then either (b) R<sup>1</sup> and R<sup>2</sup> or R<sup>5</sup> and R<sup>6</sup> are taken together to form a linkage -Q- as defined above, or (c) X is other than N, or both (b) and (c).

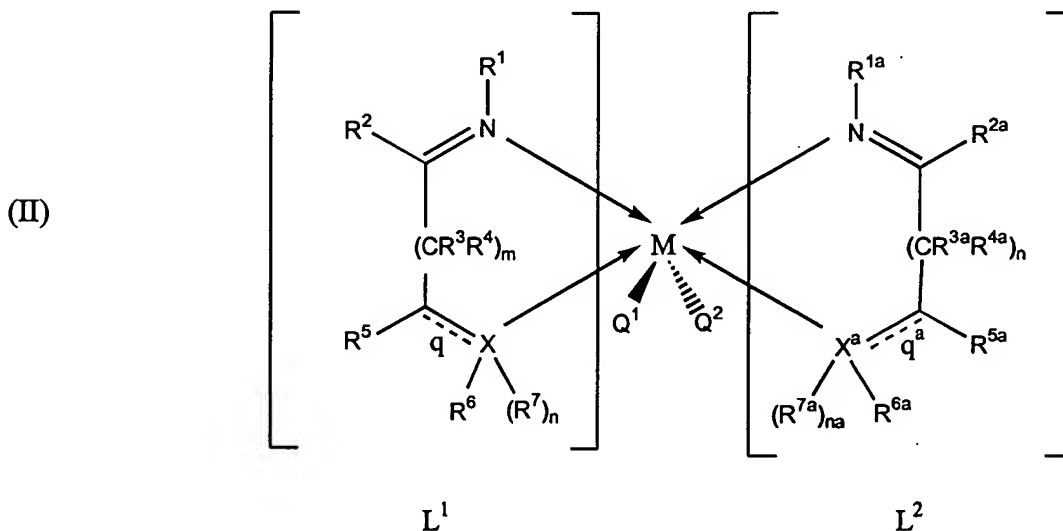
13. The compound of claim 12, wherein the compound has a positive charge +y and is associated with y/z anions each bearing a negative charge -z.

14. The compound of claim 13, wherein y and z are independently integers in the range of 1 to 4 inclusive.

15. The compound of claim 14, wherein y and z are independently 1 or 2.

16. The compound of claim 12, wherein the anions are selected from the group consisting of halide and pseudohalide.

17. The compound of claim 12, having the structure of formula (II)



wherein,  $q^a$ ,  $ma$ ,  $na$ , and  $R^{1a}$  through  $R^{7a}$  are defined as for  $q$ ,  $m$ ,  $n$  and  $R^1$  through  $R^7$ , respectively.

18. The compound of claim 17, wherein the compound has a positive charge +y and is associated with y/z anions each bearing a negative charge -z.

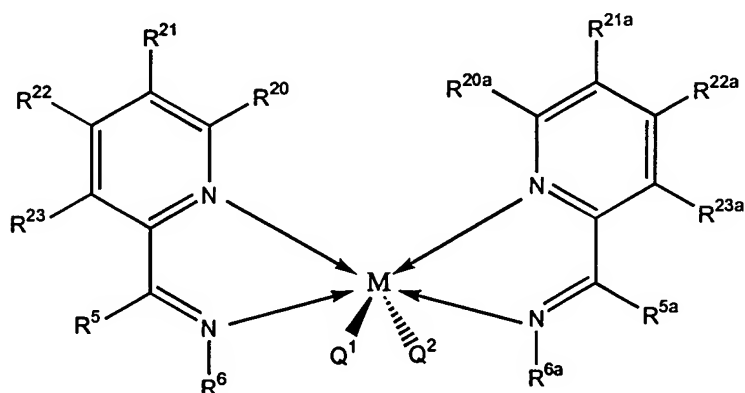
19. The compound of claim 18, wherein y and z are independently integers in the range of 1 to 4 inclusive.

20. The compound of claim 19, wherein y and z are independently 1 or 2.

21. The compound of claim 17, wherein the anions are selected from the group consisting of halide and pseudohalide.

22. The compound of claim 17, having the structure of formula (V)

(V)



wherein:

R<sup>20</sup>, R<sup>20a</sup>, R<sup>21</sup>, R<sup>21a</sup>, R<sup>22</sup>, R<sup>22a</sup>, R<sup>23</sup> and R<sup>23a</sup> are hydrido or hydrocarbyl of 1 to 10 carbon atoms, or any two adjacent R<sup>20</sup>, R<sup>20a</sup>, R<sup>21</sup>, R<sup>21a</sup>, R<sup>22</sup>, R<sup>22a</sup>, R<sup>23</sup> and R<sup>23a</sup> groups may be linked to form a five- or six-membered aromatic ring.

23. The compound of claim 22, wherein R<sup>20</sup>, R<sup>20a</sup>, R<sup>21</sup>, R<sup>21a</sup>, R<sup>22</sup>, R<sup>22a</sup>, R<sup>23</sup> and R<sup>23a</sup> are hydrido.

24. The compound of claim 22, wherein  $R^{20}$  and  $R^{20a}$  are methyl, and  $R^{21}$ ,  $R^{21a}$ ,  $R^{22}$ ,  $R^{22a}$ ,  $R^{23}$  and  $R^{23a}$  are hydrido.

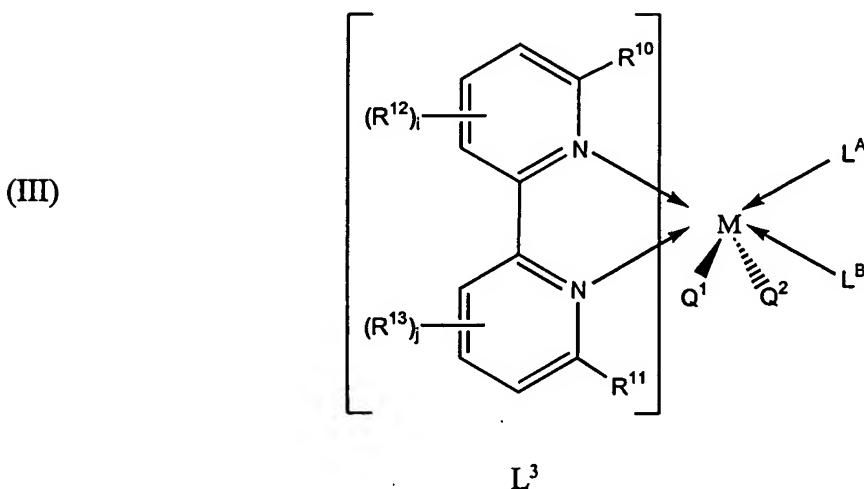
25. The compound of any one of claims 21, 22 or 23, wherein the compound has a positive charge  $+y$  and is associated with  $y/z$  anions each bearing a negative charge  $-z$ .

26. The compound of claim 25, wherein  $y$  and  $z$  are independently integers in the range of 1 to 4 inclusive.

27. The compound of claim 26, wherein  $y$  and  $z$  are independently 1 or 2.

28. The compound of claim 25, wherein the anions are selected from the group consisting of halide and pseudohalide.

29. A compound having the structure of formula (III)



wherein:

M is a mid-transition metal;

Q<sup>1</sup> and Q<sup>2</sup> are independently selected from the group consisting of hydrido, halide, alkoxy, amido, unsubstituted C<sub>1</sub>-C<sub>30</sub> hydrocarbyl, C<sub>1</sub>-C<sub>30</sub> hydrocarbyl substituted with one or more substituents such as electron-withdrawing groups, and C<sub>1</sub>-C<sub>30</sub> hydrocarbyl-substituted Group IVB elements, or Q<sup>1</sup> and Q<sup>2</sup> may together form an alkylidene olefin, acetylene, or a five- or six-membered cyclic hydrocarbyl group;

L<sup>A</sup> and L<sup>B</sup> are ligands which may be the same or different and are independently selected from the group consisting of nitrogen-containing, sulfur-containing and oxygen-containing heterocycles, tertiary amines and phosphines, or L<sup>A</sup> and L<sup>B</sup> may together form a single bidentate ligand that may or may not be the same as L<sup>3</sup>;

i and j are independently zero, 1, 2 or 3; and

R<sup>10</sup>, R<sup>11</sup>, R<sup>12</sup> and R<sup>13</sup> are independently hydrido, hydrocarbyl or substituted hydrocarbyl.

30. A catalyst system comprising the compound of any one of claims 1, 5, 7, 12, 17 or 22 and a catalyst activator effective to produce a catalytically active ionic species when combined with said compound.

31. The catalyst system of claim 30, wherein the catalyst activator is aluminum-containing or boron-containing.

32. The catalyst system of claim 31, wherein the catalyst activator is aluminum-containing.

33. The catalyst system of claim 32, wherein the catalyst activator is an organoaluminum compound.

34. The catalyst system of claim 33, wherein the catalyst activator is an alkyl aluminoxane.

35. The catalyst system of claim 34, wherein the catalyst activator is methyl aluminoxane.

36. The catalyst system of claim 31, wherein the catalyst activator is boron-containing.

37. The catalyst system of claim 36, wherein the catalyst activator is a fluorohydrocarbylboron compound.

38. The catalyst system of claim 37, wherein the catalyst activator is a fluorinated phenylborate.

39. The catalyst system of claim 30, further including an inert polymerization diluent.

40. The catalyst system of claim 39, wherein the diluent is a volatile hydrocarbon solvent.

41. A method for preparing a polymer composition, comprising:  
contacting, under polymerization conditions, an addition polymerizable monomer having at least one degree of unsaturation with the catalyst system of claim 30.

42. The method of claim 41, wherein the addition polymerizable monomer is an olefinic or vinyl monomer.

43. The method of claim 42, wherein the addition polymerizable monomer is ethylene.



44. The method of claim 42, wherein the addition polymerizable monomer is propylene.

5 45. A method for synthesizing an isotactic polyolefin, comprising:  
providing an isospecific catalyst comprising the compound of claim 5;  
admixing the catalyst with a catalyst activator, to produce a catalyst system; and  
contacting, under polymerization conditions, an olefinic monomer  $\text{CH}_2=\text{CH}_2(\text{R})$   
wherein R is other than hydrogen, with the catalyst system.

10 46. The method of claim 45, wherein R is methyl and the isotactic polyolefin is isotactic polypropylene. 351

15 47. A method for synthesizing a syndiotactic polyolefin, comprising:  
providing a syndiospecific catalyst comprising the compound of claim 7;  
admixing the catalyst with a catalyst activator, to produce a catalyst system; and  
contacting, under polymerization conditions, an olefinic monomer  $\text{CH}_2=\text{CH}_2(\text{R})$   
wherein R is other than hydrogen, with the catalyst system.

20 48. The method of claim 47, wherein R is methyl and the syndiotactic polyolefin is syndiotactic polypropylene.

25 49. A method for synthesizing linear low density polyethylene (LLDPE), comprising:  
providing a catalyst comprising the compound of claim 1;  
admixing the catalyst with a catalyst activator, to produce a catalyst system; and  
contacting, under polymerization conditions, a mixture of olefinic monomers with the  
catalyst system, wherein the mixture comprises ethylene and a second olefinic co-monomer  
 $\text{CH}_2=\text{CHR}$ , wherein R is a  $\text{C}_4\text{-C}_8$  alkyl group. 352

50. The method of claim 49, wherein the second olefinic co-monomer represents approximately 5 mole % to 15 mole % of the mixture.

51. The method of claim 50, wherein the second olefinic co-monomer is selected from the group consisting of 1-butene, 1-hexene, 1-octene, 4-methyl-1-pentene, and mixtures thereof.

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.6

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